

Fermi Liquids and the Luttinger Integral

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The Luttinger Theorem, which relates the electron density to the volume of the Fermi surface in an itinerant electron system, is taken to be one of the essential features of a Fermi liquid. The microscopic derivation of this result depends on the vanishing of a certain integral, the Luttinger integral I_L , which is also the basis of the Friedel sum rule for impurity models, relating the impurity occupation number to the scattering phase shift of the conduction electrons. It is known that non-zero values of I_L with $I_L = \pm\pi/2$, occur in impurity models in phases with non-analytic low energy scattering, classified as singular Fermi liquids. Here we show the same values, $I_L = \pm\pi/2$, occur in an impurity model in phases with regular low energy Fermi liquid behavior. Consequently the Luttinger integral can be taken to characterize these phases, and the quantum critical points separating them interpreted as topological.

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The characteristic feature of a Fermi liquid is that the low energy behavior can be understood in terms of interacting quasiparticles and their collective excitations. In the Landau formulation these are taken to be in 1-1 correspondence with those of the non-interacting system, such that the volume of the Fermi surface in the interacting system gives the electron density. Using the results of Luttinger^{1,2} in his microscopic derivation of Fermi liquid theory we can define quasiparticles which have an infinite lifetime. We consider a three dimensional lattice system with Bloch states with energy $\epsilon(\mathbf{k})$ and a single electron Green's function $G(\mathbf{k}, \omega)$ with a self-energy at zero temperature $\Sigma(\mathbf{k}, \omega)$ due to interactions. We rewrite the self-energy in the form^{3,4},

$$\Sigma(\mathbf{k}, \omega) = \Sigma(\mathbf{k}_F, 0) + \omega \Sigma'(\mathbf{k}_F, 0) + \Sigma^{\text{rem}}(\mathbf{k}, \omega), \quad (1)$$

where the Fermi wavevectors \mathbf{k}_F , and hence the Fermi surface, are defined by the condition $\epsilon(\mathbf{k}_F) + \Sigma(\mathbf{k}_F, 0) = 0$ and $\Sigma^{\text{rem}}(\mathbf{k}, \omega)$ is the remainder term. From Luttinger's results² we take the ω -derivative $\Sigma'(\mathbf{k}_F, 0)$ to be real and $\Sigma^{\text{rem}}(\mathbf{k}_F, \omega) \sim \omega^2$ as $\omega \rightarrow 0$, giving

$$G(\mathbf{k}, \omega) = \frac{z(\mathbf{k}_F)}{\omega - \tilde{\epsilon}(\mathbf{k}) - \tilde{\Sigma}(\mathbf{k}, \omega)}, \quad (2)$$

where $\tilde{\epsilon}(\mathbf{k}) = z(\mathbf{k}_F)(\epsilon(\mathbf{k}) - \epsilon(\mathbf{k}_F))$, $\tilde{\Sigma}(\mathbf{k}, \omega) = z(\mathbf{k}_F)\Sigma^{\text{rem}}(\mathbf{k}, \omega)$ and $z(\mathbf{k}_F) = (1 - \Sigma'(\mathbf{k}_F, 0))^{-1}$. We can define a free quasiparticle Green's function, $\tilde{G}_0(\mathbf{k}, \omega)$,

$$\tilde{G}_0(\mathbf{k}, \omega) = \frac{1}{\omega - \tilde{\epsilon}(\mathbf{k})}. \quad (3)$$

The Luttinger theorem is then equivalent to the statement that the total number of electrons corresponds to an integration of the *free quasiparticle* spectral density over all the states ($\tilde{\epsilon}(\mathbf{k}) < 0$) up to the Fermi level $\omega = 0$, provided the integral

$$I_L = \text{Im} \int_{-\infty}^0 \sum_{\mathbf{k}} \left(G(\mathbf{k}, \omega) \frac{\partial \Sigma(\mathbf{k}, \omega)}{\partial \omega} \right) d\omega = 0. \quad (4)$$

Essentially the same condition applies for the Friedel sum rule, which gives the number of impurity electrons n_{imp} in terms of the phase shift η of the conduction electrons⁵. For example, for the Anderson impurity model with an impurity d-level ϵ_d hybridized with conduction band electrons ϵ_k , with a hybridization matrix element V_k , this takes the form,

$$n_d = \frac{2}{\pi} \eta + \frac{2}{\pi} I_L, \quad (5)$$

where for an Anderson model with a flat wide conduction band $n_{\text{imp}} = n_d$, with

$$\eta = \frac{\pi}{2} - \tan^{-1} \left(\frac{\epsilon_d + \Sigma_R(0)}{\Delta} \right), \quad I_L = \text{Im} \int G_d(\omega) \frac{\partial \Sigma(\omega)}{\partial \omega} d\omega, \quad (6)$$

where $\Delta = \pi \sum_k |V_k|^2 \delta(\epsilon_k)$, and $G_d(\omega)$ is the impurity d-Green's function, $(G_d(\omega))^{-1} = (\omega + i\Delta \text{sgn}(\omega) - \epsilon_d - \Sigma(\omega))$, where $\Sigma_R(\omega)$ is the real part of the self-energy $\Sigma(\omega)$. The Friedel sum rule corresponds to the case⁶ where the occupation is determined entirely by the phase shift, i.e. $I_L = 0$.

The question has been raised over a number of years as to whether Luttinger's theorem holds in certain regimes of models used to describe strongly correlated electron systems⁷⁻¹². There is also recent experimental evidence¹³ in the underdoped phase of the cuprate superconductors that the volume of the Fermi surface corresponds not to the total electron number $1 - p$ but to the doping level p . Without definitive results for models of these systems the question remains open. There are, however, exact results for many impurity models where this question can be put to the test. It has been found that there are some impurity systems¹⁴, such as an underscreened Kondo model^{15,16}, and for certain parameter regimes in models of a triangular arrangement of quantum dots^{17,18}, where Eqn. (5) is only satisfied if I_L takes values $\pm\pi/2$. The low energy fixed point in a numerical renormalization group (NRG) for these systems corresponds to

free fermions, with leading irrelevant terms that are non-analytic in ω , taking the form $1/(\ln(\omega/T_K))^2$, where T_K is a Kondo temperature. As a consequence these have been classified as *singular* Fermi liquids.

We show here the existence of phases of an impurity model with the low energy behavior corresponding to well defined quasiparticles together with interaction terms that give the usual low energy frequency and temperature Fermi liquid scattering effects of order ω^2 and T^2 but with *non-zero values of the Luttinger integral*, $I_L = \pm\pi/2$.

The model we consider describes two quantum dots or impurities coupled by an antiferromagnetic exchange and direct term, with a Hamiltonian $\mathcal{H} = \sum_{\alpha=1,2} \mathcal{H}_\alpha + \mathcal{H}_{12}$, with \mathcal{H}_α corresponding to an individual Anderson impurity model with channel index α ,

$$\mathcal{H}_\alpha = \sum_{\sigma} \epsilon_{d,\alpha} d_{\alpha,\sigma}^\dagger d_{\alpha,\sigma} + \sum_{k,\sigma} \epsilon_{k,\alpha} c_{k,\alpha,\sigma}^\dagger c_{k,\alpha,\sigma} \quad (7)$$

$$+ \sum_{k,\sigma} (V_{k,\alpha} d_{\alpha,\sigma}^\dagger c_{k,\alpha,\sigma} + \text{h.c.}) + U_\alpha n_{d,\alpha,\uparrow} n_{d,\alpha,\downarrow},$$

where $d_{\alpha,\sigma}^\dagger, d_{\alpha,\sigma}$ are creation and annihilation operators for an electron at the impurity site in channel α , where $\alpha = 1, 2$, and spin component $\sigma = \uparrow, \downarrow$. The creation and annihilation operators $c_{k,\alpha,\sigma}^\dagger, c_{k,\alpha,\sigma}$ are for partial wave conduction electrons with energy $\epsilon_{k,\alpha}$ in channel α , each with a bandwidth $2D$, with $D = 1$. The Hamiltonian \mathcal{H}_{12} we take to have an antiferromagnetic exchange term J and a direct interaction U_{12} between the two impurities,

$$\mathcal{H}_{12} = 2JS_{d,1} \cdot S_{d,2} + U_{12} \sum_{\sigma,\sigma'} n_{d,1,\sigma} n_{d,2,\sigma'}. \quad (8)$$

For simplicity we consider identical dots so we can drop the index α for the impurities.

The model has been well studied, in this^{19,20} and earlier forms where the impurities are described by Kondo models^{21–26,28}. The main focus of these studies has been the quantum critical point which occurs at a critical coupling $J = J_c$ on increasing J . For $J < J_c$ any magnetic screening of the impurities is via the conduction electrons in their respective baths, but for $J > J_c$, the impurities are screened locally by the interaction between them. Here we are concerned with the phases on either side of this transition for the model away from particle-hole symmetry.

The NRG low energy fixed point and the leading irrelevant terms of this model for a Fermi liquid fixed point can be analysed by replacing the parameters ϵ_d, V_k, U, J and U_{12} , by renormalized values, $\tilde{\epsilon}_d, \tilde{V}_k, \tilde{U}, \tilde{J}$ and \tilde{U}_{12} with the additional proviso that all two-body interaction terms have to be normal ordered. Though we take $U_{12} = 0$ in all cases considered here there are finite values of \tilde{U}_{12} to be taken into account in general. The renormalized parameters (RP) can be deduced from the single particle and two-particle excitations on the approach to the fixed point as has been described elsewhere²⁷. The

phase shift η in terms of the free quasiparticles is given by

$$\eta = \frac{\pi}{2} - \tan^{-1} \left(\frac{\tilde{\epsilon}_d}{\tilde{\Delta}} \right), \quad (9)$$

from which we deduce a value for \tilde{n}_d , the total quasiparticle occupation number per impurity site, from the relation $\tilde{n}_d = 2\eta/\pi$. The results are shown in Fig. 1 as a function of J/J_c for the particular parameter set, $\epsilon_d/\pi\Delta = 0.159$, $\pi\Delta = 0.01$, and $U/\pi\Delta = 0.5$. This is compared with the total occupation value on each dot n_d as calculated directly from an NRG calculation from the expectation value of $\sum_{\sigma} d_{\sigma}^\dagger d_{\sigma}$ in the ground state. For $J < J_c$ there is a very precise agreement between the values of \tilde{n}_d and n_d . At $J = J_c$ there is a sudden jump in the value of \tilde{n}_d by 1, which corresponds to a jump in the phase shift η by $\pi/2$. This persists for $J > J_c$ such that the value of \tilde{n}_d exceeds n_d by 1. The phase shift of $\pi/2$ cannot be accounted for by a jump to another branch of the arctan; it suggests that the more general Luttinger-Friedel sum rule given in Eqn. (5) should be used in calculating \tilde{n}_d .

To test this result we carry out an alternative direct calculation of I_L using the NRG results for the self-energy and Green's function for one of the impurity sites over the same range. We can rewrite the expression for I_L in the form,

$$I_L = - \int_{-\infty}^0 \text{Im } G_d(\omega) d\omega - \frac{2}{\pi} \left[\frac{\pi}{2} - \tan^{-1} \left(\frac{\epsilon_d + \Sigma_R(0)}{\Delta} \right) \right]. \quad (10)$$

The results for n_d and $\Sigma_R(0)$ across the transition are shown in Fig. 2 for the parameter set used in Fig. 1. They show clearly that the non-zero value of the Luttinger integral I_L arises from the discontinuity in $\Sigma_R(0)$ as the value of n_d as calculated from the integral term on the right hand side of Eqn. (10) is continuous across the transition. The corresponding result for I_L is shown in Fig. 3 showing that $I_L = \pi/2$ for all values with $J > J_c$. Also shown are the results for a second parameter set, $\epsilon_d/\pi\Delta = -1.0$, $\pi\Delta = 0.01$, and $U = 0$ ($J_c = 1.5126323 \times 10^{-2}$), where the impurity level lies below the Fermi level $\epsilon_d < 0$, giving $I_L = -\pi/2$ for $J > J_c$. When taking these values into account on applying the more general Luttinger-Friedel sum rule in Eqn. (5) the relation $\tilde{n}_d = n_d$ is restored.

To test this behavior more generally we calculated I_L/π for the parameter set $J/\pi\Delta = 8$, $U/\pi\Delta = 4$, $\pi\Delta = 0.01$, and varied ϵ_d , where $J > J_c$ in all cases. The results for I_L/π are shown in Fig. 4 plotted as a function of ϵ_d . In all cases $J > J_c$, we find a constant value $I_L/\pi = 1/2$ over range $\epsilon_d < -U/2$ and $I_L/\pi = -1/2$ over range $\epsilon_d > -U/2$, where the change of sign is at the point with particle-hole symmetry. We conclude that I_L takes constant values in the different phases.

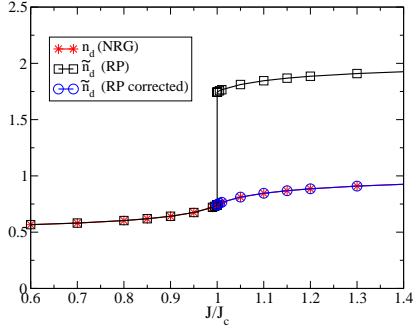


FIG. 1. (Color online) A plot of the impurity site occupation number n_d , as calculated directly from the NRG, as a function of J/J_c , compared with \tilde{n}_d (RP) from the Friedel sum rule and as corrected with the Luttinger integral, for $\epsilon_d/\pi\Delta = 0.159$, $\pi\Delta = 0.01$, $U/\pi\Delta = 0.5$ and $J_c = 5.4401763 \times 10^{-3}$.

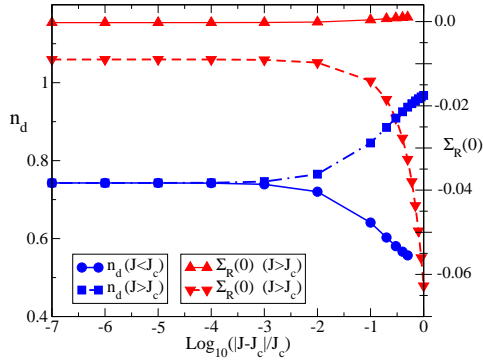


FIG. 2. (Color online) A plot of the occupation number per site n_d and the real part of the self-energy $\Sigma_R(\omega)$ at $\omega = 0$, as a function of $\text{Log}_{10}(|J - J_c|/J_c)$ for the parameter set in Fig. 1.

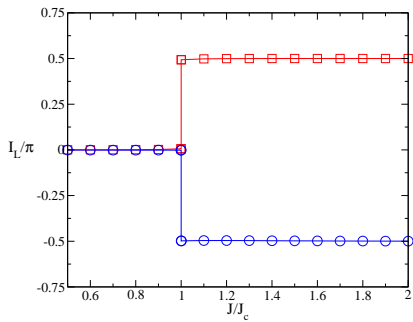


FIG. 3. (Color online) A plot of the Luttinger integral I_L/π as a function of J/J_c for the parameter set in Fig. 1 (circles) and the set, $\epsilon_d/\pi\Delta = -1.0$, $\pi\Delta = 0.01$, $U = 0$ and $J_c = 1.5126323 \times 10^{-2}$ (squares).

The jump in the phase shift of $\pi/2$, from $J_- = J_c - \delta$ to $J_+ = J_c + \delta$, $\delta \rightarrow 0^+$, from Eqn. (9) implies a

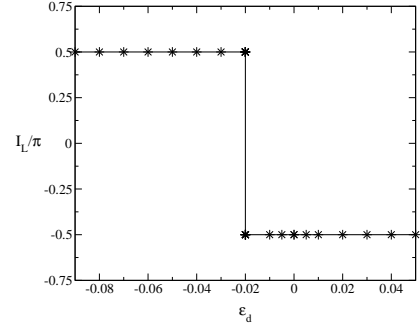


FIG. 4. (Color online) A plot of the Luttinger integral I_L/π as a function of ϵ_d for the parameter set with $J/\pi\Delta = 8$, $U/\pi\Delta = 4$ and $\pi\Delta = 0.01$.

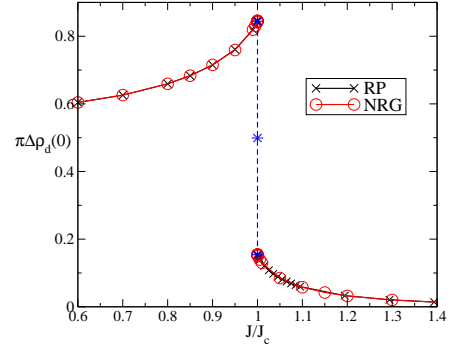


FIG. 5. (Color online) A plot of $\pi\Delta\rho_d(0)$ as a function of J/J_c for the parameter set in Fig. 1 as calculated from the renormalized parameters (crosses) and from the NRG calculated spectral density (circles).

discontinuity in $\tilde{\epsilon}_d/\tilde{\Delta}$ such that

$$\left(\frac{\tilde{\epsilon}_d}{\tilde{\Delta}}\right)_+ \left(\frac{\tilde{\epsilon}_d}{\tilde{\Delta}}\right)_- = -1, \quad (11)$$

or equivalently a discontinuity in the value of $\Sigma(0)$. In the Luttinger-Friedel sum rule this is compensated by the jump in the Luttinger integral to $\pm\pi/2$, so that the value of n_d is continuous through the transition. The sudden discontinuity in $\Sigma(0)$ is however reflected in the spectral density of states $\rho_d(\omega)$ at the impurity site at the Fermi level $\omega = 0$. In terms of the phase shift $\rho_d(0)$ is given by

$$\rho_d(0) = \frac{\sin^2(\eta)}{\pi\Delta} = \frac{1}{\pi\Delta} \frac{\tilde{\Delta}^2}{\tilde{\epsilon}_d^2 + \tilde{\Delta}^2}. \quad (12)$$

We can calculate this quantity from Eqn. (12) using renormalized parameters as deduced from the low energy fixed point or directly from the self-energy $\Sigma(\omega)$ as calculated via the NRG. In Fig. 5 we give the results for $\pi\Delta\rho_d(0)$ as a function of J/J_c for the parameter set in Fig. 1. We see complete agreement between the two sets of results, confirming the interpretation of the state in the

regime $J > J_c$ as a Fermi liquid. The mid-point of the discontinuity, indicated by a star in Fig 5, corresponds to $\rho_d(0) = 1/2\pi\Delta$, and seems to be a general feature independent of the particular parameter set chosen.

Apart from the sudden jump in the value of $\rho_d(0)$ at $J = J_c$, there is a continuous redistribution of the spectral weight $\rho_d(\omega)$ as J varies through the transition region. In Fig. 6 we show this change for the parameter set in Fig. 1 by comparing the forms for $\rho_d(\omega)$ for $J/J_c = 0.8, 0.99, 1.01, 1.2$. For $J = 0.8J_c$ there is a single broad peak above the Fermi level, which becomes very narrow and shifts to just above the Fermi level at $J = 0.99J_c$. After the transition for $J = 1.01J_c$ there is a sudden drop in the spectral density at the Fermi level and a peak just below the Fermi level. For $J = 1.2J_c$ the peak has shifted to lower energies and broadened with a distinct local minimum in $\rho_d(\omega)$ at the Fermi level. The form of the spectral density in the immediate region of the Fermi level is to a good approximation given by the spectral density due to the free quasiparticles, $\tilde{\rho}_d(\omega) = \tilde{\Delta}/\pi((\omega - \tilde{\epsilon}_d)^2 + \tilde{\Delta}^2)$, when multiplied by the quasiparticle weight factor $z = \tilde{\Delta}/\Delta$, reflecting the Fermi liquid nature of the low lying excitations. As $J \rightarrow J_c$, $\tilde{\epsilon}_d \rightarrow 0$ and $\tilde{\Delta} \rightarrow 0$, this quasiparticle expression gives the narrowing of the peak on the approach to the transition. The discontinuity in $\tilde{\epsilon}_d$ at $J = J_c$ and change of sign from Eqn. (11) gives the shift of the peak across the Fermi level.

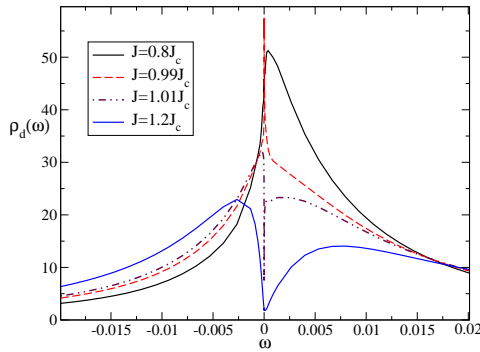


FIG. 6. (Color online) A plot of $\rho_d(\omega)$ as a function of ω for the parameter set in Fig. 1 with values of $J/J_c = 0.8, 0.99, 1.01, 1.2$.

Finally in Fig. 7 we give the imaginary part of the self-energy $\Sigma(\omega)$ as a function of ω/T^* , where T^* is the renormalized energy scale $T^* = \pi\tilde{\Delta}/4$. Here for Fermi liquid behavior, as in the single impurity Anderson model, we expect an ω^2 form on the scale $\omega < T^*$. There are some inaccuracies in calculating this quantity from an NRG calculation due to broadening of discrete data, but there is a very reasonable fit to the quadratic form as given in the plot.

We have established that in this model, away from particle-hole symmetry, we have three Fermi liquid

phases. Only one of them has the expected value $I_L = 0$ for the Luttinger integral. The other two have constant values of I_L with $I_L = \pi/2$ or $I_L = -\pi/2$. As the case with $I_L = 0$ includes the case $J = 0$ and the single impurity Anderson model, it fits the condition in some definitions of a Fermi liquid that the states of the interacting system correspond to an adiabatic evolution from those of the non-interacting system. This is not the case for the phases with $I_L = \pm\pi/2$, but nevertheless they satisfy all the other usual requirements of a Fermi liquid; well defined low energy quasiparticles, with non-singular scattering leading to the usual ω^2 terms, and consequent T^2 low temperature behavior. The case with particle-hole symmetry is different. Though there is a sudden change of phase shift by $\frac{\pi}{2}$ at $J = J_c$, for $J > J_c$ we find the self-energy has a simple pole, $\Sigma(\omega) \sim \frac{1}{\omega}$ as $\omega \rightarrow 0$, and consequently the spectral density goes to zero at the Fermi level.

The Wilson ratios for a spin, charge, staggered spin and charge, in the Fermi liquid regimes on both sides of the transition at $J = J_c$ were calculated in earlier work^{19,20} from the renormalized parameters for the quasiparticles, and were in complete agreement with exact results found in essentially the same model studied by De Leo and Fabrizio²⁸.

The different Fermi liquid phases can be classified by the quantum number $2I_L/\pi$, which is not associated with any symmetry. This could give a general explanation as to puzzling question as to why the transition in this model is so robust, existing not only away from particle-hole symmetry but also for $U = 0$. As this quantum number cannot change continuously at any transition between these phases, it implies that the transition at $J = J_c$ is essentially a topological one. Our results also raise the question as to whether the Luttinger integral can take similar values and modify the standard Luttinger relation in strong correlation lattice models, such as the t-J model.

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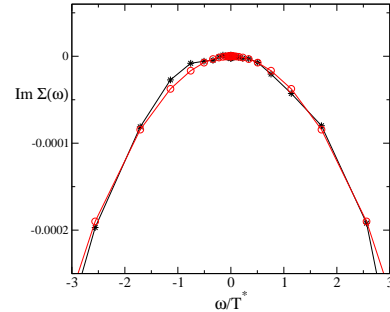


FIG. 7. (Color online) A plot of $\text{Im}\Sigma(\omega)$ as a function of ω/T^* for the parameter set in Fig. 1 from the NRG results (stars) with a quadratic fit (circles) for $J = 2J_c$ and $T^* = \pi\tilde{\Delta}/4 = 9.14553 \times 10^{-5}$.

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